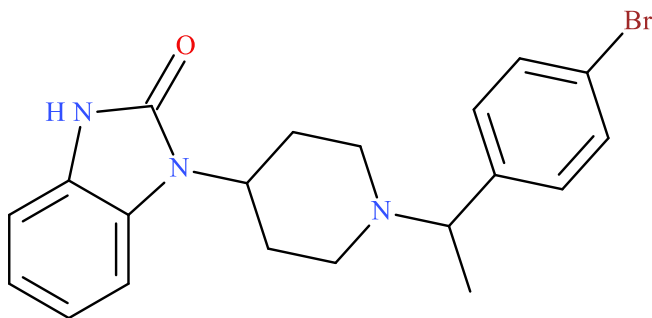


## Brorphine

Sample Type: **Biological Fluid**

Latest Revision: **July 17, 2020**

Date of Report: **July 17, 2020**



### 1. GENERAL INFORMATION

|                      |   |
|----------------------|---|
| <b>IUPAC Name:</b>   | 3-[1-[1-(4-bromophenyl)ethyl]-4-piperidyl]-1H-benzimidazol-2-one  |
| <b>InChI String:</b> | InChI=1S/C20H22BrN3O/c1-14(15-6-8-16(21)9-7-15)23-12-10-17(11-13-23)24-19-5-3-2-4-18(19)22-20(24)25/h2-9,14,17H,10-13H2,1H3,(H,22,25) |
| <b>CFR:</b>          | Not Scheduled (07/2020)   |
| <b>CAS#</b>          | Not Available   |
| <b>Synonyms:</b>     | Not Available   |
| <b>Source:</b>       | NMS Labs – Toxicology Department  |

**Important Note:** All identifications were made based on evaluation of analytical data (LC-QTOF-MS) in comparison to analysis of acquired reference material.

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## 2. CHEMICAL AND PHYSICAL DATA

### 2.1 CHEMICAL DATA

| Form | Chemical Formula                                   | Molecular Weight | Molecular Ion [M <sup>+</sup> ] | Exact Mass [M+H] <sup>+</sup> |
|------|--|------------------|---------------------------------|-------------------------------|
| Base | C <sub>20</sub> H <sub>22</sub> BrN <sub>3</sub> O | 400.3            | 399                             | 400.1019                      |

### 3. BRIEF DESCRIPTION

Brorphine is classified as a novel opioid. Novel opioids have been reported to cause psychoactive effects similar to heroin, fentanyl, and other opioids. Novel opioids have also caused adverse events, including deaths, as described in the literature. It is unclear when brorphine was first synthesized or how it received its name, but literature regarding brorphine and structurally similar analogues exists.<sup>1,2,3</sup> Emerging *in vitro* data show that brorphine exhibits potency similar to that of fentanyl.<sup>4,5</sup> Brorphine may be considered structurally similar to fentanyl, however, its structure differs from previously identified fentanyl analogues and would not constitute scheduling under core-structure regulation of fentanyl-related substances. Therefore, brorphine is not a scheduled substance in the United States. Identifications of brorphine have now been reported in the United States and Europe (Belgium).

### 4. ADDITIONAL RESOURCES

1. Janssen, P.A.J. (1964) Derivatives of benzimidazoliny piperidine. US3318900A. <https://patents.google.com/patent/US3318900A/en>
2. Kawamoto, H., Ozaki, S., Itoh, Y., Miyaji, M., Arai, S., Nakashima, H., Kato, T., Ohta, H., Iwasawa (1999) Discovery of the first potent and selective small molecule opioid receptor-like (ORL1) antagonist: 1-[(3R,4R)-1-cyclooctylmethyl-3-hydroxymethyl-4-piperidyl]-3-ethyl-1,3-dihydro-2H-benzimidazol-2-one (J-113397). *Journal of Medicinal Chemistry*, **42**, 5061-5063.
3. Kennedy, N.M., Schmid, C.L., Ross, N.C., Lovell, K.M., Yue, Z., Chen, Y.T., Cameron, M.D., Bohn, L.M., Bannister, T.D. (2018) Optimization of a series of mu opioid receptor (MOR) agonists with high G protein signaling bias. *Journal of Medicinal Chemistry*, **61**, 8895-8907.
4. Verougstraete, N., Vandeputte, M., Lyphout, C., Cannaert, A., Hulpia, F., Van Calenbergh, S., Verstraete, A., Stove, C. (2020) First report on brorphine: the next opioid on the deadly new psychoactive substances' horizon? *Journal of Analytical Toxicology*. [Epub ahead of print]

5. Vandeputte, M.M., Cannaert, A., Stove, C.P. (2020) *In vitro* functional characterization of a panel of non-fentanyl opioid new psychoactive substances. *Archives of Toxicology*. DOI: 10.1007/s00204-020-02855-7

[https://www.caymanchem.com/product/27816/brorphine-\(hydrochloride\)](https://www.caymanchem.com/product/27816/brorphine-(hydrochloride))

## 5. QUALITATIVE DATA

### 5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

**Testing Performed At:** NMS Labs (Willow Grove, PA)

**Sample Preparation:** Acid/base extraction

**Instrument:** Agilent 5975 Series GC/MSD System

**Standard:** Reference material for Brorphine (Batch: 0567046-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). ([https://www.caymanchem.com/product/27816/brorphine-\(hydrochloride\)](https://www.caymanchem.com/product/27816/brorphine-(hydrochloride)))

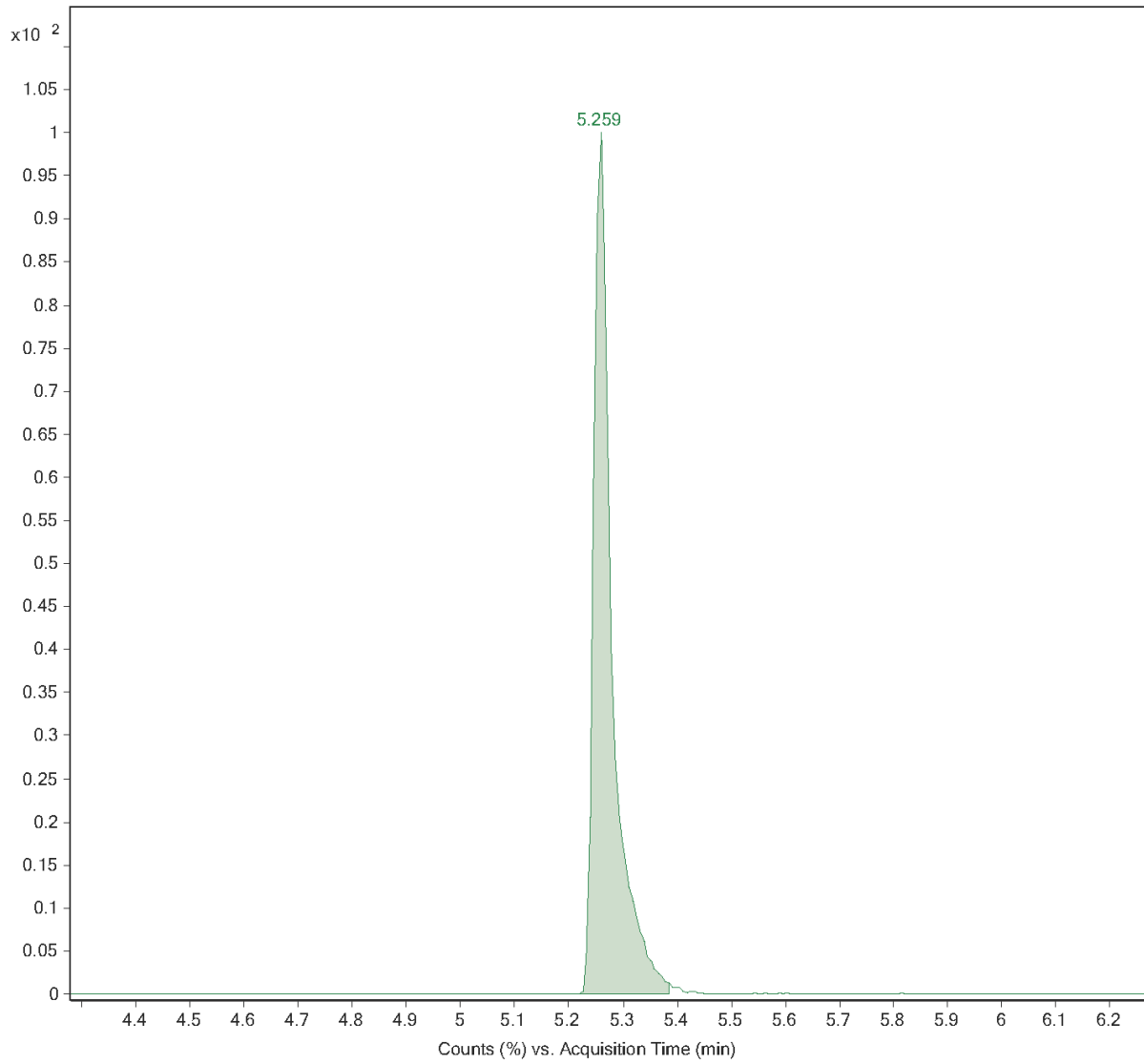
#### EI (70 eV) Mass Spectrum: Brorphine (Standard)



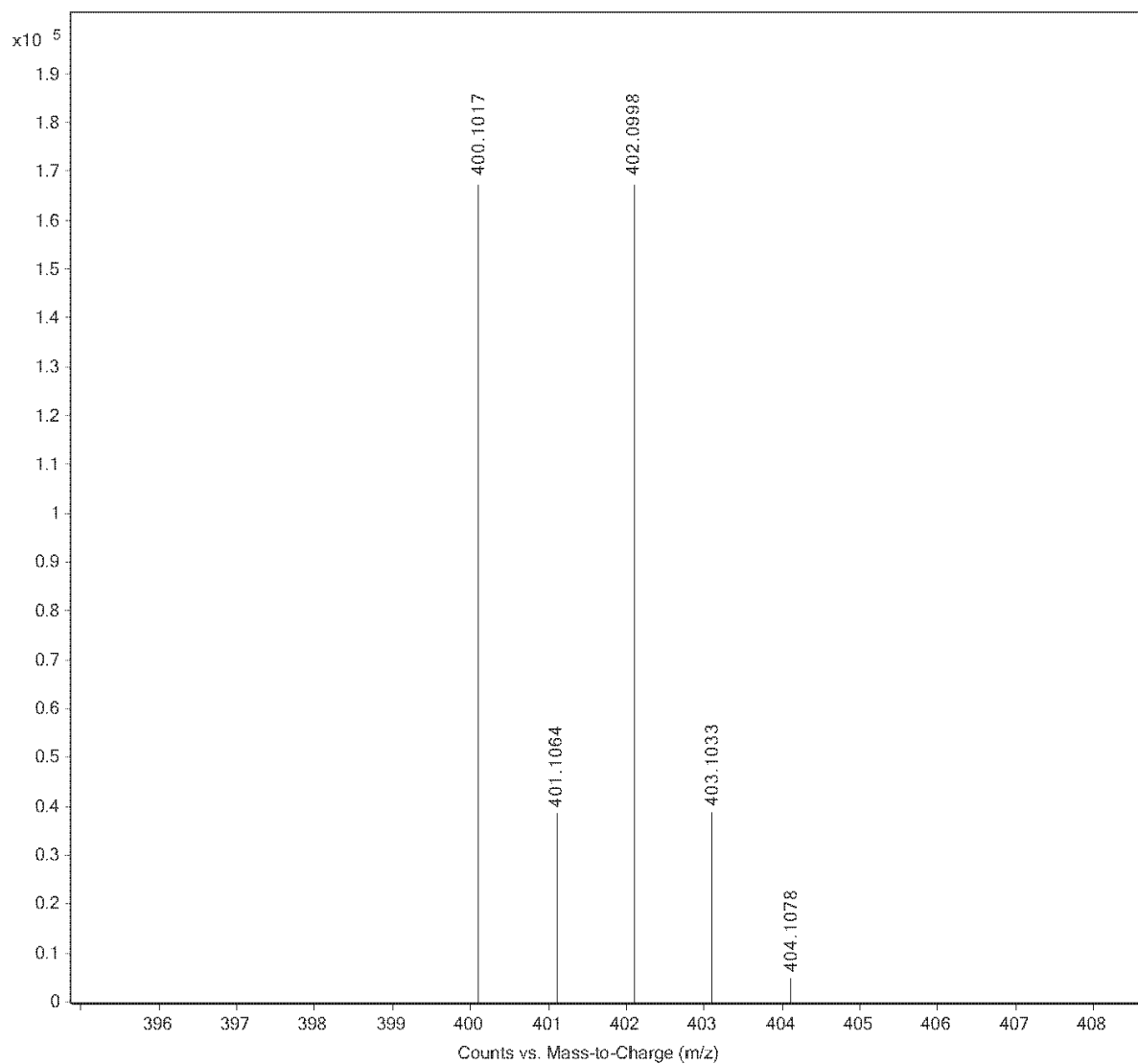
## 5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY (LC-QTOF-MS)

|                              |   |
|------------------------------|---|
| <b>Testing Performed At:</b> | NMS Labs (Horsham, PA)  |
| <b>Sample Preparation:</b>   | Liquid-liquid extraction  |
| <b>Instrument:</b>           | Agilent Technologies 6230 LC-TOF-MS   |
| <b>Column:</b>               | Zorbax Eclipse Plus C18 Rapid Resolution HT (3x100mm, 1.8 $\mu$ m)  |
| <b>Mobile Phase:</b>         | A: Ammonium formate (5 mM, 0.05% formic acid)<br>B: Methanol (0.05% formic acid)<br>Flow rate: 0.7 mL/min   |
| <b>Gradient:</b>             | Initial: 95A:5B; 3A:97B over 7.25 min; 95A:5B at 8.25 min   |
| <b>Temperatures:</b>         | Autosampler: 15 °C<br>Column Oven: 55 °C  |
| <b>Injection Parameters:</b> | Injection Volume: 5 $\mu$ L   |
| <b>TOF Parameters:</b>       | TOF MS Scan Range: 100 and 1000 Da  |
| <b>Retention Time:</b>       | 5.259 min   |
| <b>Standard Comparison:</b>  | Reference material for Brorphine (Batch: 0567046-2) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the extract as Brorphine, based on retention time (5.276 min) and mass spectral data.<br><a href="https://www.caymanchem.com/product/27816/brorphine-hydrochloride">https://www.caymanchem.com/product/27816/brorphine-hydrochloride</a> |

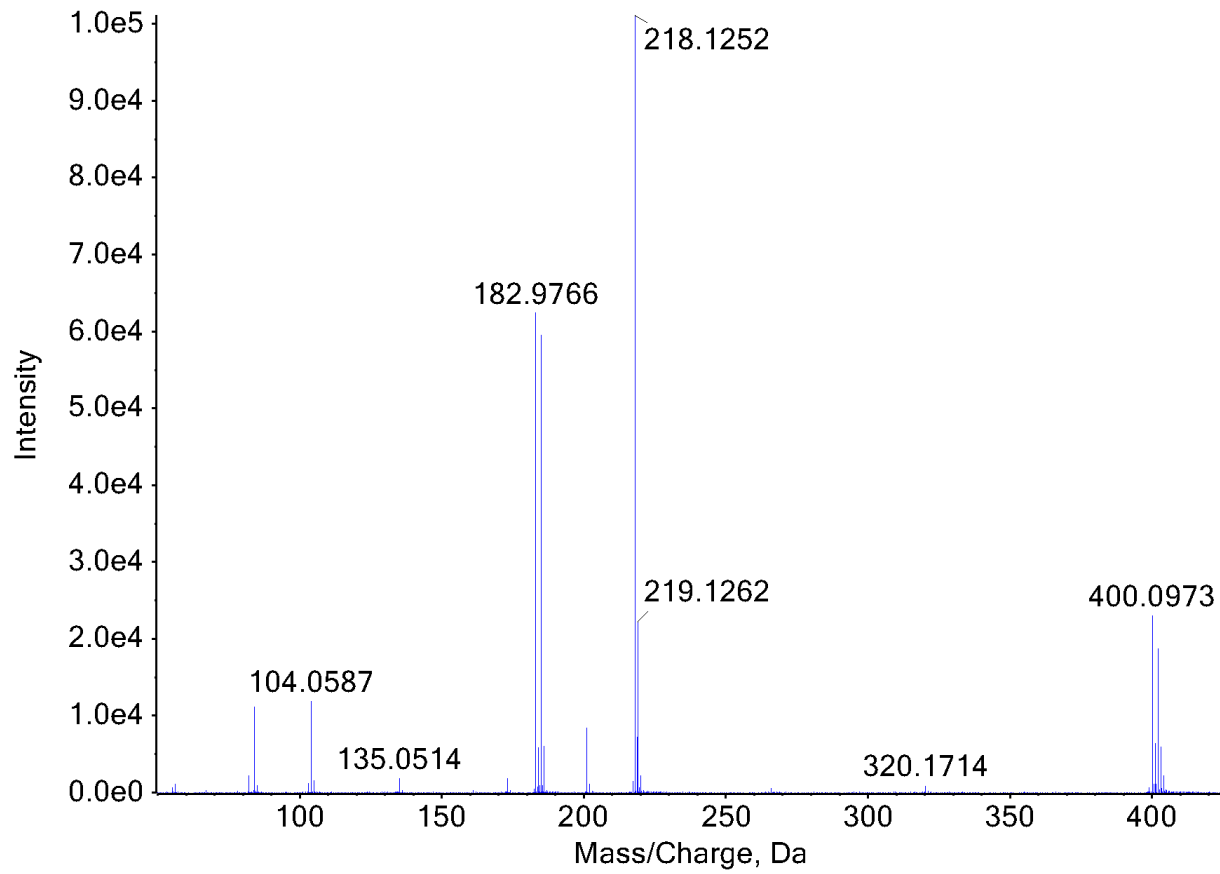
### Extracted Ion Chromatogram (XIC): Brorphine (Blood Specimen)



### TOF MS Spectrum: Brorphine (Blood Specimen)



**LC-QTOF-MS\* – MS/MS Spectrum: Brorphine (Standard)**



*\*Acquired at the Center for Forensic Science Research and Education (CFSRE)  
using a SCIEX TripleTOF® 5600+*